

chain nodes:

7 8 9 10 11 12 13 15 16 18 19

ring nodes:

1 2 3 4 5 6

chain bonds:

1-7 1-11 2-8 2-10 4-6 4-19 5-12 5-13 8-9 13-15 13-16 13-18

ring bonds:

1-2 1-5 2-3 3-4 4-5

exact/norm bonds:

1-2 1-5 1-7 2-3 3-4 4-5 4-6 13-15 13-16 13-18

exact bonds:

1-11 2-8 2-10 4-19 5-12 5-13 8-9

G1:H,F

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS12:CLASS13:CLASS 15:CLASS16:CLASS18:CLASS19:CLASS

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

```
LOGINID: sspta1600txm
PASSWORD:
LOGINID/PASSWORD REJECTED
The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.
Do you wish to retry the logon?
Enter choice (y/N):
Do you wish to use the same loginid and password?
Enter choice (y/N):
Enter new loginid (or press [Enter] for sspta1600txm):
Enter new password:
LOGINID:
LOGINID:ssspta1600txm
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2
* * * * * * * * *
                      Welcome to STN International
NEWS
                  Web Page URLs for STN Seminar Schedule - N. America
      1
 NEWS
                  "Ask CAS" for self-help around the clock
      2
 NEWS
      3
         FEB 27
                  New STN AnaVist pricing effective March 1, 2006
 NEWS
      4
         APR 04
                  STN AnaVist $500 visualization usage credit offered
                 CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS
      5
         MAY 10
 NEWS
      6 MAY 11
                  KOREAPAT updates resume
 NEWS
      7
         MAY 19
                  Derwent World Patents Index to be reloaded and enhanced
 NEWS
      8 MAY 30
                  IPC 8 Rolled-up Core codes added to CA/CAplus and
                  USPATFULL/USPAT2
NEWS 9 MAY 30
                  The F-Term thesaurus is now available in CA/CAplus
 NEWS 10
         JUN 02
                  The first reclassification of IPC codes now complete in
                  INPADOC
NEWS 11
         JUN 26
                  TULSA/TULSA2 reloaded and enhanced with new search and
                  and display fields
NEWS 12
          JUN 28
                  Price changes in full-text patent databases EPFULL and PCTFULL
 NEWS 13
         JUl 11
                  CHEMSAFE reloaded and enhanced
 NEWS 14
         JUl 14
                  FSTA enhanced with Japanese patents
 NEWS 15
         JUl 19
                 Coverage of Research Disclosure reinstated in DWPI
 NEWS 16
         AUG 09
                  INSPEC enhanced with 1898-1968 archive
 NEWS EXPRESS
               JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(jP),
               AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.
 NEWS HOURS
               STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN
               Welcome Banner and News Items
```

NEWS IPC8 For general information regarding STN implementation of IPC 8 NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 13:59:47 ON 09 AUG 2006

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:00:24 ON 09 AUG 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 AUG 2006 HIGHEST RN 899769-93-8 DICTIONARY FILE UPDATES: 8 AUG 2006 HIGHEST RN 899769-93-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10608907.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR G1 H, F

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam SAMPLE SEARCH INITIATED 14:00:47 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1 TO 80 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d scan 12

L2 1 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 9H-Purin-2-amine, 6-chloro-9-[(2R)-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]- (9CI)

MF C11 H13 C1 F N5 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 full sss

FULL SEARCH INITIATED 14:01:09 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS

26 ANSWERS

SEARCH TIME: 00.00.01

L3 26 SEA SSS FUL L1

=> d 1-26 13

L3ANSWER 1 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN

892389-31-0 REGISTRY Entered STN: 12 Jul 2006 ED

CN INDEX NAME NOT YET ASSIGNED

FS STEREOSEARCH

MF C12 H14 F2 N4 O4

SR

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3ANSWER 2 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 892389-29-6 REGISTRY

ED Entered STN: 12 Jul 2006

CN INDEX NAME NOT YET ASSIGNED

FS STEREOSEARCH

MF C12 H15 F2 N5 O3

SR

LCSTN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 3 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 892389-27-4 REGISTRY
- ED Entered STN: 12 Jul 2006
- CN INDEX NAME NOT YET ASSIGNED
- FS STEREOSEARCH
- MF C16 H16 C1 F2 N3 O5
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 4 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 892389-10-5 REGISTRY
- ED Entered STN: 12 Jul 2006
- CN INDEX NAME NOT YET ASSIGNED
- FS STEREOSEARCH
- MF C12 H14 F2 N4 O3
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 881881-89-6 REGISTRY
- ED Entered STN: 26 Apr 2006
- CN 9H-Purin-2-amine, 6-chloro-9-[(2R)-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C11 H13 C1 F N5 O3
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 6 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 881881-88-5 REGISTRY
- ED Entered STN: 26 Apr 2006
- CN 9H-Purin-2-amine, 6-chloro-9-[(2R)-3,5-di-O-acetyl-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C15 H17 C1 F N5 O5
- SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 881881-83-0 REGISTRY
- ED Entered STN: 26 Apr 2006
- CN 9H-Purin-2-amine, 6-chloro-9-[(2R)-3,5-di-O-acetyl-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]-N-(triphenylmethyl)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C34 H31 C1 F N5 O5
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 879551-07-2 REGISTRY
- ED Entered STN: 07 Apr 2006
- CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-bis(2,2-

dimethylpropanoate), (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H34 F N3 O7

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 874638-98-9 REGISTRY

ED Entered STN: 20 Feb 2006

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H18 F N3 O5

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 10 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 874638-97-8 REGISTRY

ED Entered STN: 20 Feb 2006

CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C32 H26 F N5 O6

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 874638-95-6 REGISTRY

ED Entered STN: 20 Feb 2006

CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H18 F N5 O4

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 874638-94-5 REGISTRY
- Entered STN: 20 Feb 2006 ED
- CN Benzamide, N- $[1-[(2R)-3,5-di-O-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-\alpha-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-deoxy-2-fluoro-2-methyl-a-D-benzoyl-2-fluoro-2$ erythro-pentofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C31 H26 F N3 O7
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- ANSWER 13 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN RN 874638-82-1 REGISTRY
- ED Entered STN: 20 Feb 2006
- Benzamide, N-[1-[(2R)-5-O-benzoyl-2-deoxy-2-fluoro-2-methyl-3-O-

McIntosh

L3

(methylsulfonyl)- β -D-erythro-pentofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H24 F N3 O8 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 14 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 863329-66-2 REGISTRY

ED Entered STN: 16 Sep 2005

CN Uridine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H13 F N2 O5

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN RN 863329-65-1 REGISTRY

ED Entered STN: 16 Sep 2005

CN Uridine, 2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H21 F N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 16 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 818374-78-6 REGISTRY

ED Entered STN: 21 Jan 2005

CN Adenosine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 F N5 O3

CI COM

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-45-8 REGISTRY

ED Entered STN: 20 Jan 2005

CN Guanosine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 F N5 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 18 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-44-7 REGISTRY

ED Entered STN: 20 Jan 2005

CN Cytidine 5'-(tetrahydrogen triphosphate), 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H17 F N3 O13 P3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-43-6 REGISTRY

ED Entered STN: 20 Jan 2005

CN Adenosine, 2'-deoxy-2'-fluoro-2'-methyl-, monohydrochloride, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 F N5 O3 . C1 H

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CRN (818374-78-6)

Absolute stereochemistry.

● HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-42-5 REGISTRY

ED Entered STN: 20 Jan 2005

CN 9H-Purine, 6-chloro-9-[(2R)-2-deoxy-2-fluoro-2-methyl- β -D-erythropentofuranosyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H12 C1 F N4 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-41-4 REGISTRY

ED Entered STN: 20 Jan 2005

CN 9H-Purine, 6-chloro-9-[(2R)-3,5-di-O-acetyl-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H16 C1 F N4 O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-38-9 REGISTRY

ED Entered STN: 20 Jan 2005

CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, monohydrochloride, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H14 F N3 O4 . C1 H

SR CA

LC STN Files: CA, CAPLUS, PROUSDDR, TOXCENTER, USPATFULL

CRN (817204-33-4)

Absolute stereochemistry. Rotation (+).

● HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN
- RN
- 817204-37-8 REGISTRY Entered STN: 20 Jan 2005 ED
- CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'bis(trifluoroacetate), (2'R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C21 H16 F7 N3 O7
- SR
- LCSTN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN RN 817204-33-4 REGISTRY

ED Entered STN: 20 Jan 2005

CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H14 F N3 O4

CI COM

SR CA

LC STN Files: CA, CAPLUS, PROUSDDR, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 817204-32-3 REGISTRY

ED Entered STN: 20 Jan 2005

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H26 F N3 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2006 ACS on STN

RN 510765-38-5 REGISTRY

ED Entered STN: 05 May 2003

CN Uridine, 2'-deoxy-2'-fluoro-2'-(hydroxymethyl)-3-[(2-methoxyethoxy)methyl], (2'S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C14 H21 F N2 O8

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 216.78 216.99

FULL ESTIMATED COST

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http://www.cas.org/infopolicy.html

=> d his (FILE 'HOME' ENTERED AT 13:59:47 ON 09 AUG 2006) FILE 'REGISTRY' ENTERED AT 14:00:24 ON 09 AUG 2006 L1STRUCTURE UPLOADED L2 1 S L1 SSS SAM L3 26 S L1 FULL SSS FILE 'CAPLUS' ENTERED AT 14:01:32 ON 09 AUG 2006 7 L3 L4=> d bib abs hitstr 1-7 14 L4ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN AN 2006:603846 CAPLUS DN 145:76603 TIFluorinated pyrrolo[2,3-d]pyrimidine nucleosides for the treatment of RNA-dependent RNA viral infection Maccoss, Malcolm; Olsen, David B.; Leone, Joseph; Durette, Philippe L. ΙN Merck & Co., Inc., USA PA PCT Int. Appl., 46 pp. SO CODEN: PIXXD2 DT Patent LA English FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ----**-**PΙ WO 2006065335 A2 20060622 WO 2005-US37224 20051017 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM PRAI US 2004-620743P P 20041021 US 2005-651366P Ρ 20050209 AB The present invention provides fluorinated pyrrolo[2,3, d]pyrimidine nucleoside compds. which are inhibitors of RNA-dependent RNA viral polymerase. These compds. are inhibitors of RNA-dependent RNA viral replication and are useful for the treatment of RNA-dependent RNA viral infection. They are particularly useful as precursors to inhibitors of hepatitis C virus (HCV) NS5B polymerase, as precursors to inhibitors of HCV replication, and/or for the treatment of hepatitis C infection. The invention also describes pharmaceutical compns. containing such fluorinated pyrrolo[2,3-d]pyrimidine nucleoside alone or in combination with other agents active against RNA-dependent RNA viral infection, in particular HCV infection. Also disclosed are methods of inhibiting RNA-dependent RNA

polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the fluorinated

pyrrolo[2,3-d]pyrimidine nucleoside of the present invention. IT 892389-29-6 892389-31-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(fluorinated pyrrolopyrimidine nucleosides for treatment of RNA-dependent RNA viral infection)

RN 892389-29-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 892389-31-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

IT 892389-27-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorinated pyrrolopyrimidine nucleosides for treatment of RNA-dependent RNA viral infection)

RN 892389-27-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

IT 892389-10-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (fluorinated pyrrolopyrimidine nucleosides for treatment of RNA-dependent RNA viral infection)

RN 892389-10-5 CAPLUS

INDEX NAME NOT YET ASSIGNED CN

Absolute stereochemistry.

ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN 2006:269477 CAPLUS L4

ΑN

144:312289 DN

Preparation of alkyl-substituted 2-deoxy-2-fluoro-D-ribofuranosyl TΙ pyrimidine and purine nucleoside analogs via condensation of the lactone to nucleosides as potential antiviral agents

IN Chun, Byoung-Kwon; Wang, Peiyuan

PΑ

Pharmasset, Inc., USA PCT Int. Appl., 74 pp. SO

CODEN: PIXXD2

DTPatent

English LA

FAN.CNT 1

	PATENT NO.					KIND		DATE		APPLICATION NO.						DATE		
							_											
ΡI	WO 2006031725				A2		20060323		WO 2005-US32406						20050913			
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               GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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     US 2006122146
                               A1
                                      20060608
                                                    US 2005-225425
                                                                                20050913
PRAI US 2004-609783P
                               Ρ
                                      20040914
      US 2004-610035P
                               Ρ
                                      20040915
      US 2005-666230P
                               Ρ
                                      20050329
OS
     MARPAT 144:312289
GΙ
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AΒ A process for preparing of 2-deoxy-2-fluoro-2-methyl-D-ribonolactones, I, wherein R1 and R2 can independently be H, CH3, acetyl, benzoyl, pivaloyl, 4-nitrobenzoyl, 3-nitrobenzoyl, 2-nitrobenzoyl, 4-chlorobenzoyl, 3-chlorobenzoyl, 2-chlorobenzoyl, 4-methylbenzoyl, 3-methylbenzoyl, 2-methylbenzoyl, 4-phenylbenzoyl, benzyl, 4-methoxybenzyl, trityl, trialkylsilyl, t-butyl-dialkylsilyl, t-butyldiphenylsilyl, TIPDS, THP, MOM, or MEM are prepared and used in the condensation to 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs. Thus, 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs II and III, wherein X is a halogen; Y is N or CH; Z is a halogen, hydroxyl, ether, thiol, thioether, (un) substituted amine or alkyl; R1' is alkyl, vinyl, ethynyl; R2' and R3' can be same or different H, alkyl, arylalkyl, acyl, cyclic acetal such as 2',3'-O-isopropylidene or 2',3-O-benzylidene, or 2',3'-cyclic carbonate; R4, R5, and R6 are independently H, halogen, hydroxyl, ether, thiol, thioether, N3, (un) substituted amine, (un) substituted amido, alkyl, halogenated alkyl, alkenyl, halogenated alkenyl, alkynyl, halogenated alkynyl, hydroxy alkyl, alkoxy are prepared and are potential anti-HCV agents. Specifically, IV was prepared in 88 % yield via condensation, alkylation and stereoselective fluorination reactions and can exhibit potential use as an anti-HCV agent. ΙT 879551-07-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of alkyl-substituted 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs via condensation of the lactone to nucleosides)

RN 879551-07-2 CAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-bis(2,2-dimethylpropanoate), (2'R)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:128527 CAPLUS

DN 144:370341

TI Synthesis and antiviral activity of 2'-deoxy-2'-fluoro-2'-C-methyl purine nucleosides as inhibitors of hepatitis C virus RNA replication

AU Clark, Jeremy L.; Mason, J. Christian; Hollecker, Laurent; Stuyver, Lieven J.; Tharnish, Phillip M.; McBrayer, Tamara R.; Otto, Michael J.; Furman, Phillip A.; Schinazi, Raymond F.; Watanabe, Kyoichi A.

CS Pharmasset, Inc., Tucker, GA, 30084, USA

SO Bioorganic & Medicinal Chemistry Letters (2006), 16(6), 1712-1715

CODEN: BMCLE8; ISSN: 0960-89/4X

PB Elsevier B.V.

DT Journal LA English

OS CASREACT 144:370341

GΙ

AB A series of purine nucleosides, e.g. I, containing the 2'-deoxy-2'-fluoro-2'-C-methylribofuranosyl moiety were synthesized and evaluated as potential inhibitors of the hepatitis C virus in vitro. Of the nucleosides that were synthesized, only those possessing a 2-amino group on the purine base reduced the levels of HCV RNA in a sub-genomic replicon assay.

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antiviral activity of deoxyfluoromethyl purine

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10/608,907
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nucleosides as inhibitors of hepatitis C virus RNA replication)

RN 881881-89-6 CAPLUS

CN 9H-Purin-2-amine, 6-chloro-9-[(2R)-2-deoxy-2-fluoro-2-methyl-β-D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 817204-42-5P 817204-45 8P 818374-78-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

(synthesis and antiviral activity of deoxyfluoromethyl purine nucleosides as inhibitors of hepatitis C virus RNA replication)

RN 817204-42-5 CAPLUS

CN 9H-Purine, 6-chlorg-9-[(2R)-2-deoxy-2-fluoro-2-methyl-β-D-erythro-pentofuranosyl]- (βCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 817204-45-8 CAPLUS

CN Guanosine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

Absolute steredchemistry.

C1
N
N
N
R
R
R
OAC
OAC

RN 881881-83-0 CAPLUS

CN 9H-Purin 2-amine, 6-chloro-9-[(2R)-3,5-di-O-acetyl-2-deoxy-2-fluoro-2-methyl-6 D-erythro-pentofuranosyl]-N-(triphenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 881881-88-5 CAPLUS

9H-Purin-2-amine, 6-chloro-9-[(2R)-3,5-di-0-acetyl-2-deoxy-2-fluoro-2-methyl- β -D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 10 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
L4
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ΑN 2006:103884 CAPLUS

DN 144:171198

Preparation of alkyl-substituted 2-déoxy-2-fluoro-D-ribofuranosyl ΤI pyrimidine and purine nucleoside análogs via condensation of the lactone to nucleosides as potential antiviral agents Wang, Peiyuan; Stec, Wojciech; Clark, Jeremy; Chun, Byoung-Kwon; Shi,

IN

PA

Junxing; Du, Jinfa Pharmasset, Inc., USA PCT Int. Appl., 34 pp. SO

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT	KIND DATE			APPLICATION NO.						DATE						
	/ /															
				WO 2005-US25916						20050721						
W:	ΑE,	AG,	AL,	AM,	ÁΤ,	AU/,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
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	LC,	LK,	LR,	LS/	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,
				/												
				/												
	WO 2006	W: AE, CN, GE,	WO 2006012440 W: AE, AG, CN, CO, GE, GH,	WO 2006012440 W: AE, AG, AL, CN, CO, CR, GE, GH, GM,	WO 2006012440 A2 W: AE, AG, AL, AM, CN, CO, CR, CU, GE, GH, GM, HR,	WO 2006012440 A2 W: AE, AG, AL, AM, AT, CN, CO, CR, CU, CZ, GE, GH, GM, HR, HU,	WO 2006012440 A2 2006 W: AE, AG, AL, AM, AT, AU, CN, CO, CR, CU, CZ, DE, GE, GH, GM, HR, HU, ID,	WO 2006012440 A2 20060202 W: AE, AG, AL, AM, AT, AU, AZ, CN, CO, CR, CU, CZ, DE, DK, GE, GH, GM, HR, HU, ID, IL,	WO 2006012440 A2 20060202 W: AE, AG, AL, AM, AT, AU, AZ, BA, CN, CO, CR, CU, CZ, DE, DK, DM, GE, GH, GM, HR, HU, ID, IL, IN,	WO 2006012440 A2 20060202 WO 2 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, GE, GH, GM, HR, HU, ID, IL, IN, IS,	WO 2006012440 A2 20060202 WO 2005- W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,	WO 2006012440 A2 20060202 WO 2005-US25 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE,	WO 2006012440 A2 20060202 WO 2005-US25916 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,	WO 2006012440 A2 20060202 WO 2005-US25916 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM,	WO 2006012440 A2 20060202 WO 2005-US25916 20 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP,	

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      US 2005277598
                                  A1
                                                          US 2005-118613
                                                                                        20050429
PRAI US 2004-589866P
                                  Ρ
                                          20040/721
                                          2004/0909
      US 2004-608320P
                                  Ρ
      US 2004-566584P
                                  Ρ
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OS
      MARPAT 144:171198
GΙ
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

A process for preparing of 2-deoxy-2-fluoro-2-methyl-D-ribonolactones, I, wherein R1 and R2 can independently be H, CH3, acetyl, benzoyl, pivaloyl, 4-nitrobenzoyl, 3-nitrobenzoyl, 2-nitrobenzoyl, 4-chlorobenzoyl, 3-chlorobenzoyl, 2-chlorobenzoyl, 4-methylbenzoyl, 3-methylbenzoyl, 4-phenylbenzoyl, benzyl, 4-methoxybenzyl, trityl, trialkylsilyl, t-butyl-dialkylsilyl, t-butyldiphenylsilyl, TIPDS, THP, MOM, or MEM are prepared and used in the condensation to 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs. Thus, 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs II and III, wherein X is a halogen; Y is N or CH; Z is a halogen, hydroxyl, ether, thiol, thioether, (un) substituted amine or alkyl; R1' is alkyl, vinyl, ethynyl; R2' and R3' can be same or different H, alkyl, arylalkyl, acyl, cyclic acetal such as 2',3'-O-isopropylidene or 2',3-O-benzylidene, or 2',3'-cyclic carbonate; R4, R5, and R6 are independently H, halogen, hydroxyl, ether, thiol, thioether, N3, (un) substituted amine, (un) substituted amido, alkyl, halogenated alkyl, alkenyl, halogenated alkenyl, alkynyl, halogenated alkynyl, hydroxy alkyl, alkoxy are prepared and are potential anti-HCV agents. Specifically, IV was prepared (no yield, claimed) via condensation, alkylation and stereoselective fluorination reactions and can exhibit potential use as an anti-HCV agent.

IT 874638-97-8P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of alkyl-substituted 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs via condensation of the lactone to nucleosides)

RN 874638-97-8 CAPLUS

CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

IT 817204-32-3P 817204-33-4P 874638-82-1P 874638-94-5P 874638-95-6P 874638-98-9P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of alkyl-substituted 2-deoxy-2-fluoro-D-ribofuranosyl pyrimidine and purine nucleoside analogs via condensation of the lactone to nucleosides)

RN 817204-32-3 CAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 817204-33-4 CAPLUS CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 874638-82-1 CAPLUS

CN Benzamide, N-[1-[(2R)-5-O-benzoyl-2-deoxy-2-fluoro-2-methyl-3-O-(methylsulfonyl)- β -D-erythro-pentofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 874638-94-5 CAPLUS

CN Benzamide, N-[1-[(2R)-3,5-di-O-benzoyl-2-deoxy-2-fluoro-2-methyl- α -D-erythro-pentofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 874638-95-6 CAPLUS

CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

RN 874638-98-9 CAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:648160 CAPLUS

DN 143:248607

TI Design, Synthesis, and Antiviral Activity of 2'-Deoxy-2'-fluoro-2'-C-methyl-cytidine, a Potent Inhibitor of Hepatitis C Virus Replication

AU Clark, Jeremy L.; Hollecker, Laurent; Mason, J. Christian; Stuyver, Lieven J.; Tharnish, Phillip M., Lostia, Stefania; McBrayer, Tamara R.; Schinazi, Raymond F.; Watanabe, Kyoichi A.; Otto, Michael J.; Furman, Phillip A.; Stec, Wojciech J.; Patterson, Steven E.; Pankiewicz, Krzysztof W.

CS Pharmasset, Inc., Princeton, NJ, 08540, USA

SO Journal of Medicinal Chemistry (2005), 48(17), 5504-5508 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

The pyrimidine nucleoside- β -D-2'-deoxy-2'-fluoro-2'-C-methylcytidine (I) was designed as a hepatitis C virus RNA-dependent RNA polymerase (HCV RdRp) inhibitor. The title compound was obtained by a DAST fluorination of N4-benzoyl-1-(2-methyl-3,5-di-O-benzoyl- β -D-arabinofuranosyl)cytosine to provide N4-benzoyl-1-(2-fluoro-2-methyl-3,5-di-O-benzoyl- β -D-ribofuranosyl)cytosine. The protected 2'-C-methylcytidine was obtained as a byproduct from the DAST fluorination and allowed for the preparation of two biol. active compds. from a common precursor. Compound I and 2'-C-methylcytidine were assayed in a sub-genomic HCV replicon assay

RN 817204-32-3 CAPLUS
CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3
(2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 863329-65-1 CAPLUS

CN Uridine, 2'-deoxý-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 817204-38-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (design, synthesis via fluorination, and antiviral activity of 2'-deoxy-2'-fluoro-2'-C-methyl-cytidine, a potent inhibitor of Hepatitis C virus replication)

RN $817204 - \beta 8 - 9$ CAPLUS

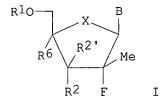
CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, monohydrochloride, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:34765 CAPLUS
ΑN
     142:94074
DN
ΤI
     Preparation of modified fluorinated (2'R)-2'-deoxy-2'-fluoro-2'-C-methyl
     nucleoside analogs as antiviral agents
IN
     Clark, Jeremy
PΑ
     Pharmasset, Ltd., Barbados
SO
     PCT Int. Appl., 228 pp.
     CODEN: PIXXD2
DT
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LA
     English
FAN.CNT 1
     PATENT NO.
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                                 DATE
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                                                                     DATE
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             TD, TG
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                                                                     20040421
     EP 1633766
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                                 20060315
                                             EP 2004-775900
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV,
                             FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-474368P
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                                20030530
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     WO 2004-US12472
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OS
     MARPAT 142:94074
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AB The disclosed invention provides nucleoside analogs I, wherein B is purine and pyrimidine nucleobase; X is O, S, CH2, Se, NH, N-alkyl, CHW, C(W)2; W is F, Cl, Br, iodo; Rl is H, phosphate, H-phosphonate, acyl, Ph, alkyl, carboxyalkylamino, sulfonate ester, peptide, amino acid, sugar reside; R2 and R2' are independently H, alkyl, alkenyl, alkynyl, vunyl, N3, CN,

halogen, NO2, ester, alkoxy, thioalkyl, sulfoxide, sulfonyl; R6 is alkyl, CN, Me, OMe, OEt, CH2OH, CH2F, N3, CHCN, CH2N3, CH2NH2, CH2NHMe, CH2NMe2, alkylne; and methods of treating a Flaviviridae infection, including hepatitis C virus, West Nile Virus, yellow fever virus, and a rhinovirus infection in a host, including animals, and especially human, using a (2'R)-2'-deoxy-2'-fluoro-2'-C-Me nucleosides, or a pharmaceutically acceptable salt or prodrug thereof. Thus, (2'R)-2'-deoxy-2'-fluoro-2'-C-methylcytidine was prepared and tested as antiviral agent. The effects the nucleoside analogs tested on human bone marrow cells are reported. (2'R)-2'-deoxy-2'-fluoro-2'-C-methylcytidine shows activity against Rhinovirus, West Nile virus, Yellow Fever virus, and Dengue virus. Cytotoxicity and effect of nucleoside analogs on human bone marrow cells are reported.

IT 817204-33-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of modified fluorinated (2'R)-2'-deoxy-2'-fluoro-2'-C-Me nucleoside analogs as antiviral agents)

RN 817204-33-4 CAPLUS

CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 817204-38-9P 817204-42-5P 817204-43-6P 817204-45-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of modified fluorinated (2'R)-2'-deoxy-2'-fluoro-2'-C-Me nucleoside analogs as antiviral agents)

RN 817204-38-9 CAPLUS

CN Cytidine, 2'-deoxy-2'-fluoro-2'-methyl-, monohydrochloride, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RN 817204-42-5 CAPLUS

CN 9H-Purine, 6-chloro-9-[(2R)-2-deoxy-2-fluoro-2-methyl- β -D-erythropentofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 817204-43-6 CAPLUS

CN Adenosine, 2'-deoxy-2'-fluoro-2'-methyl-, monohydrochloride, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 817204-45-8 CAPLUS
CN Guanosine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

IT 817204-44-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(preparation of modified fluorinated (2'R)-2'-deoxy-2'-fluoro-2'-C-Me nucleoside analogs as antiviral agents)

RN 817204-44-7 CAPLUS

Absolute stereochemistry.

IT 817204-32-3P 817204-37-8P 817204-41-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of modified fluorinated (2'R)-2'-deoxy-2'-fluoro-2'-C-Me nucleoside analogs as antiviral agents)

RN 817204-32-3 CAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-dibenzoate, (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 817204-37-8 CAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro-2'-methyl-, 3',5'-bis(trifluoroacetate), (2'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 817204-41-4 CAPLUS

CN 9H-Purine, 6-chloro-9-[(2R)-3,5-di-O-acetyl-2-deoxy-2-fluoro-2-methyl-β-D-erythro-pentofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:114368 CAPLUS

DN 138:304462

TI Synthesis of 2'-C- β -Fluoromethyluridine

AU Dai, Qing; Piccirilli, Joseph A.

- CS Howard Hughes Medical Institute, Department of Biochemistry & Molecular Biology, Department of Chemistry, The University of Chicago, Chicago, IL, 60637, USA
- SO Organic Letters (2003), 5(6), 807-810 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 138:304462
- AB 2'-C- β -Fluoromethyluridine represents both a potentially important biol. agent and a tool for biochem. anal. Here the authors describe the first synthesis of this compound starting from uridine. The key steps include protection of the uracil base with methoxyethoxymethyl (MEM) chloride, conversion to the corresponding 2'-C- α -epoxide, and regioselective opening of the oxirane ring with potassium fluoride/hydrogen fluoride. Subsequent acetylation of the 3'- and 5'-hydroxyl groups enables MEM removal using B-bromocatecholborane. Deacetylation generates the parent nucleoside, 2'-C- β -fluoromethyluridine.
- IT 510765-38-5P

RL: BYP (Byproduct); PREP (Preparation) (synthesis of $C-\beta$ -fluoromethyluridine from uridine via uracil protection with MEM, epoxidn. and regionelective ring opening)

RN 510765-38-5 CAPLUS

CN Uridine, 2'-deoxy-2'-fluoro-2'-(hydroxymethyl)-3-[(2-methoxyethoxy)methyl]-, (2'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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              AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.
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                  (15176-29-1/RN)
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                  (69123-90-6/RN)
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              90-2/BI)
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L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-2-fluoro- β -D-arabinofuranosyl)-

5-iodo- (9CI) MF C9 H11 F I N3 O4

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Nucleotidyltransferase, deoxyribonucleate (9CI)

MF Unspecified

CI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro- β -D-arabinofuranosyl)-5-methyl- (9CI)

MF C10 H13 F N2 O5

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Uridine, 2'-deoxy-5-ethyl- (8CI, 9CI)

MF C11 H16 N2 O5

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,4(1H,3H)-Pyrimidinedione, 1-[2-deoxy-2-fluoro-5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]- β -D-arabinofuranosyl]-5-methyl- (9CI)

MF C10 H16 F N2 O14 P3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Triphosphoric acid, P-[2-[(2-amino-1,6-dihydro-6-oxo-9H-purin-9-

yl)methoxy]ethyl] ester (9CI) MF C8 H14 N5 O12 P3 CI COM

$$H_2N$$
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 H_2N
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L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro- β -D-arabinofuranosyl)-5-ethyl- (9CI)
MF C11 H15 F N2 O5

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 12 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro- β -D-arabinofuranosyl)-5-iodo- (9CI)

MF C9 H10 F I N2 O5

CI COM